

Generalized Virial Theorem and Pressure Relation for a strongly correlated Fermi gas

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Abstract

For a two-component Fermi gas in the unitarity limit (ie, with infinite scattering length), there is a well-known virial theorem, first shown by J. E. Thomas et al, Phys. Rev. Lett. 95, 120402 (2005). A few people rederived this result, and extended it to few-body systems, but their results are all restricted to the unitarity limit. Here I show that there is a generalized virial theorem for FINITE scattering lengths. I also generalize an exact result concerning the pressure, first shown in cond-mat/0508320, to the case of imbalanced populations.

Key words: virial theorem, pressure, momentum distribution
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Two-component ultracold atomic Fermi gases with large scattering lengths have been realized recently, and have become a focus of numerous research activities. In this paper we study two exact properties of such a system.

We will consider the zero-range interaction model only, in which the scattering length a between the \uparrow and \downarrow spin states is the only parameter for the interaction. (Such a model is justified by typical experimental setups, in which the interatomic distance, the thermal de Broglie wavelength, and a are all large compared to the Van de Waals range of the interaction.)

1 Generalized Virial Theorem

If the system is confined by a harmonic trap, and is in the unitarity limit ($a \rightarrow \infty$), the total energy E is related to the external potential energy by

$$E = 2E_V. \quad (1)$$

The result (1) was first shown by J. E. Thomas et al using the local density approximation [1]. A few people rederived this result, and extended it to few-body systems, but their results are all restricted to the unitarity limit and to a harmonic confinement potential [2].

Here I show that there is a *generalized* virial theorem for *finite* scattering lengths. I also consider a somewhat more general confinement potential,

$$V(\mathbf{r}) = r^\beta f(\hat{\mathbf{r}})$$

satisfying $\beta > -2$, $\beta \neq 0$, and $\beta f(\hat{\mathbf{r}}) > 0$, where $f(\hat{\mathbf{r}})$ is any smooth function of the unit direction vector $\hat{\mathbf{r}}$. For a harmonic trap $\beta = 2$.

Such a generalized virial theorem is

$$E - \frac{\beta + 2}{2} E_V = -\frac{\hbar^2 \mathcal{I}}{8\pi a m}, \quad (2)$$

where m is the fermion mass, $\mathcal{I} = \lim_{k \rightarrow \infty} k^4 \rho_{\mathbf{k}\sigma}$, and $\rho_{\mathbf{k}\sigma}$ is the momentum distribution at momentum $\hbar \mathbf{k}$ and spin state σ . The amplitude of $\rho_{\mathbf{k}\sigma}$ is defined by $\int \frac{d^3 k}{(2\pi)^3} \rho_{\mathbf{k}\sigma} = N_\sigma$, the number of spin- σ fermions. Note that N_\uparrow and N_\downarrow are arbitrary and may be different.

\mathcal{I} equals the quantity ΩC in Refs. [3,4]. An equivalent definition of \mathcal{I} is given in Ref. [4]:

$$\mathcal{I} = \lim_{K \rightarrow \infty} \pi^2 K N_{k>K},$$

where $N_{k>K}$ is the expectation of the total number of fermions with momenta larger than $\hbar K$.

We will give \mathcal{I} a short name: *total contact*, or simply *contact*. We will give the spatial function $C(\mathbf{r})$ introduced in Ref. [3] a name: *local contact density*. The quantity $C = \Omega^{-1} \mathcal{I} = \Omega^{-1} \int d^3 r C(\mathbf{r})$ [3] will be called *average contact density* (over volume Ω). For a homogeneous system of volume Ω , $C(\mathbf{r})$ equals C .

To prove (2), we first consider an energy eigenstate ϕ at scattering length a , with energy $E = E_{\text{internal}} + E_V$, where E_{internal} is the internal energy expectation value. We then modify this state infinitesimally, in two consecutive steps.

In the first step, we adiabatically change the scattering length to $a' = (1 + \epsilon)a$, where ϵ is an infinitesimal number. The energy changes to $E' = E'_{\text{internal}} + E'_V$. Using the adiabatic sweep theorem of Ref. [4], we find

$$E' - E = \frac{\hbar^2 \mathcal{I}}{4\pi a m} \epsilon + O(\epsilon^2).$$

In the second step, we do a geometric compression of the system's wave func-

tion, from $\phi'(\mathbf{r}_1, \dots, \mathbf{r}_N)$ to

$$\phi''(\mathbf{r}_1, \dots, \mathbf{r}_N) = (1 + \epsilon)^{3N/2} \phi'((1 + \epsilon)\mathbf{r}_1, \dots, (1 + \epsilon)\mathbf{r}_N).$$

Using the short-range boundary condition for the wave function ($\phi \propto 1/s - 1/\text{scatt.length}$ when the distance s between two fermions in different spin states is small), we find that ϕ'' corresponds to a state with scattering length $a'' = a'/(1 + \epsilon) = a$. Using the energy theorem [3], we get $E''_{\text{internal}} = (1 + \epsilon)^2 E'_{\text{internal}}$, and $E''_V = (1 + \epsilon)^{-\beta} E'_V$. So

$$E'' - E' = 2\epsilon E'_{\text{internal}} - \beta\epsilon E'_V + O(\epsilon^2) = 2\epsilon E_{\text{internal}} - \beta\epsilon E_V + O(\epsilon^2).$$

Because the state ϕ'' has the *same* scattering length as the initial state ϕ , and because the difference between the two states is of the order ϵ , the variational stability of energy levels implies that $E'' - E = O(\epsilon^2)$, or $(E'' - E') + (E' - E) = O(\epsilon^2)$. So

$$\frac{\hbar^2 \mathcal{I}}{4\pi a m} + 2E_{\text{internal}} - \beta E_V = 0.$$

Rewriting $E_{\text{internal}} = E - E_V$, we get (2).

Obviously, (2) is also valid for any statistical ensemble of energy levels, with a statistical weight decaying sufficiently fast at large energy, such that \mathcal{I} equals the statistical average of the values of \mathcal{I} 's for the individual energy levels [3]. Thus (2) is valid for any finite temperature states in the canonical or grand canonical ensemble, as well as the ground state.

When $k_F a \rightarrow 0^-$ (k_F fixed), $\mathcal{I} \propto a^2$ and Eq. (2) reduces to the virial theorem for the noninteracting Fermi gas.

When $a = \infty$ and $\beta = 2$, Eq. (2) reduces to Eq. (1).

When $N_{\uparrow} = N_{\downarrow} \gg 1$, $k_F a \rightarrow 0^+$ and the temperature is zero, the system approaches a Bose-Einstein condensate of tightly bound molecules, and (2) approaches the virial theorem for the Gross-Pitaevskii equation for these bosonic molecules [5] with scattering length $a_m \approx 0.6a$ [6].

2 Pressure Relation

Suppose that the system is in a cubic box of size $L = \Omega^{1/3}$, and a periodic boundary condition is imposed. In the absence of the external potential

$$P - \frac{2}{3}\rho E = \frac{\hbar^2 C}{12\pi a m}, \quad (3)$$

where $\rho_E = E/\Omega$ is the average energy density, and $C = \mathcal{I}/\Omega$ is the average contact density. Equation (3) is valid for any energy eigenstate, or any statistical ensemble of them, with a statistical weight decaying sufficiently fast at large energy, such that \mathcal{I} equals the statistical average of the values of \mathcal{I} 's for the individual energy levels [3]. This includes any finite temperature states in the canonical or grand canonical ensemble, as well as the ground state.

In Ref. [4], the pressure relation (3) is shown for balanced populations of the two spin states: $N_\uparrow = N_\downarrow$.

Here I point out that (3) remains valid *even if* $N_\uparrow \neq N_\downarrow$. This incorporates many interesting possibilities, in particular phase separation between superfluid and normal phase [7] and, consequently, spontaneous spatial inhomogeneity of the energy density and contact density.

The general proof of (3) is very similar to that of (2). Starting with any energy eigenstate ϕ with scattering length a and energy E , we first increase the scattering length adiabatically, from a to $a' = (1 + \epsilon)a$, to get $E' = E + \frac{\hbar^2 \mathcal{I}}{4\pi am} \epsilon + O(\epsilon^2)$. We then do a geometric compression of the wave function, after which the scattering length changes back to a , the period of the wave function becomes $L/(1 + \epsilon)$, the energy becomes

$$E'' = (1 + \epsilon)^2 E' = E' + 2\epsilon E' + O(\epsilon^2) = E + \frac{\hbar^2 \mathcal{I}}{4\pi am} \epsilon + 2\epsilon E + O(\epsilon^2),$$

and the quantum state becomes ϕ'' .

If we start from the state ϕ , and compress the box by a linear factor $(1 + \epsilon)$ adiabatically, without changing the scattering length, we will get the *same* final state as ϕ'' . So the pressure is

$$P = \lim_{\epsilon \rightarrow 0} \frac{E'' - E}{\Omega - (1 + \epsilon)^{-3} \Omega} = \frac{2E}{3\Omega} + \frac{\hbar^2 \mathcal{I}}{12\pi am \Omega}.$$

Although Eq. (3) is only exact in the absence of external potential, it is approximately valid for each local part of the fermionic cloud in a trap, within the local density approximation. In this latter case, ρ_E is replaced by the local internal energy density, and C is replaced by the local contact density $C(\mathbf{r})$.

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References

- [1] J. E. Thomas, J. Kinast, A. Turlapov, Phys. Rev. Lett. 95 (2005) 120402.
- [2] F. Chevy (unpublished); F. Werner and Y. Castin, Phys.Rev.A 74 (2006) 053604; D. T. Son, arXiv:0707.1851v1; T. Mehen, arXiv:0712.0867v1.
- [3] Shina Tan, cond-mat/0505200.
- [4] Shina Tan, cond-mat/0508320.
- [5] F. Dalfovo, S. Giorgini, L. P. Pitaevskii, S. Stringari, Rev. Mod. Phys. 71 (1999) 463.
- [6] D. S. Petrov, C. Salomon, G. V. Shlyapnikov, Phy. Rev. Lett. 93 (2004) 090404.
- [7] M. W. Zwierlein, A. Schirotzek, C. H. Schunck, and W. Ketterle, Science 311 (2006) 492 ; G. B. Partridge, W. Li, R. I. Kamar, Y. Liao, and R. G. Hulet, Science 311 (2006) 503 ; Y. Shin, M. W. Zwierlein, C. H. Schunck, A. Schirotzek, and W. Ketterle, Phys. Rev. Lett. 97 (2006) 030401; G. B. Partridge, W. Li, Y. Liao, R. G. Hulet, M. Haque, and H. T. C. Stoof, Phys. Rev. Lett. 97 (2006) 190407; Y. Shin, C. H. Schunck, A. Schirotzek, and W. Ketterle, Nature, in print (arXiv:0709.3027).